

MSDE

Molecular Systems Design & Engineering rsc.li/molecular-engineering

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2058-9689 CODEN MSDEBG 8(9) 1089-1222 (2023)



Cover
See Michael Badawi *et al.*,
pp. 1165–1181.
Image reproduced by permission
of Ioannis Karamanis,
Hubert Monnier &
Michael Badawi from *Mol. Syst.
Des. Eng.*, 2023, 8, 1165.

EDITORIAL

1095

New Editor-in-Chief and Deputy Editor-in-Chief for MSDE: reflections and vision

Claire S. Adjiman* and Andrew L. Ferguson*

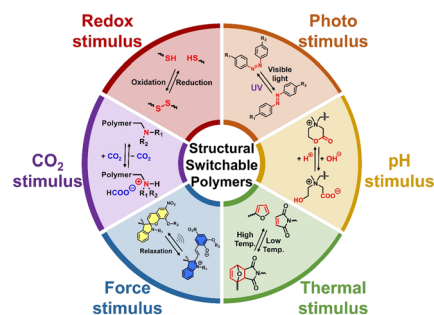


REVIEW

1097

Stimuli-responsive structure–property switchable polymer materials

Zhuang Mao Png, Chen-Gang Wang,
Jayven Chee Chuan Yeo, Johnathan Joo Cheng Lee,
Nayli Erdeanna Surat'man, Yee Lin Tan, Hongfei Liu,
Pei Wang, Beng Hoon Tan, Jian Wei Xu,* Xian Jun Loh*
and Qiang Zhu*



Editorial Staff

Executive Editor

Maria Southall

Deputy Editor

Bianca Provost

Editorial Production Manager

Chris Goodall

Assistant Editors

Sean Browner, Molly Colgate, Paul Scott, Alison Winder

Editorial Assistant

Basita Javeed

Publishing Assistant

Allison Holloway

Publisher

Sam Keltie

For queries about submitted papers, please contact

Emily Skinner, Editorial Production Manager in the first instance.

E-mail: molecularengineering@rsc.org

For pre-submission queries please contact

Maria Southall, Executive Editor.

E-mail: molecularengineering-rsc@rsc.org

MSDE (electronic: ISSN 2058-9689) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail: orders@rsc.org

2023 Annual (electronic) subscription price: £2211; \$3649.

Customers in Canada will be subject to a surcharge to cover GST.

Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017;

E-mail: advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

MSDE

Molecular Systems Design & Engineering

rsc.li/molecular-engineering

Building and designing systems from the molecular level

Editorial Board

Editor-in-Chief

Claire S. Adjiman, Imperial College London, UK

Deputy Editor-in-Chief

Andrew Ferguson, University of Chicago

Associate Editors

Luke Connal, Australian National University, Australia

Robert Riggleman, University of Pennsylvania, USA

Members

Linda Broadbelt, Northwestern University, USA
LaShanda Korley, University of Delaware, USA

Yongye Liang, Southern University of Science and Technology, China

Anja Palmans, Eindhoven University of Technology, The Netherlands

Patrick Stayton, University of Washington, USA

Advisory Board

Alfredo Alexander-Katz, MIT, USA

Helena Azevedo, Queen Mary University of London, UK

Andre Bardow, ETH Zurich, Switzerland

Jeremy Baumberg, University of Cambridge, UK

Eva Blasco, Heidelberg University, Germany

Joao Cabral, Imperial College London, UK

Neil Champness, University of Nottingham, UK

Paulette Clancy, John Hopkins University, USA

Marc-Olivier Coppens, UCL, UK

Graeme Day, University of Southampton, UK

Andrew deMello, ETH Zurich, Switzerland

Juan de Pablo, University of Chicago, USA

Cecile Dreiss, Kings College London, UK

Thomas Epps III, University of Delaware, USA

Lei Fang, Texas A&M University, USA

C. Daniel Frisbie, University of Minnesota, USA

Xuefeng Guo, Peking University, China

Kristi Kiick, University of Delaware, USA

Raju Kumar Gupta, Indian Institute of Technology

Kanpur, India

Sarah Heilshom, Stanford University, USA

Arthi Jayaraman, University of Delaware, USA

Takashi Kato, University of Tokyo, Japan

Sang Ouk Kim, KAIST, Republic of Korea

Jodie Lutkenhaus, Texas A&M University, USA

Heidi Mansour, University of Arizona, USA

Bert Meijer, Eindhoven University of Technology,

Netherlands

Takashi Nakanishi, NIMS, Japan

Ki Tae Nam, Seoul National University, Republic

of Korea

Insup Noh, Seoul National University of Science &

Technology, Republic of Korea

Mark A. Olson, Tianjin University, China

Ho Bum Park, Hanyang University, South Korea

Jon Parquette, Ohio State University, USA

Boaz Pokroy, Technion – Israel Institute of

Technology, Israel

Jeffrey Rimer, University of Houston, USA

Shu Seki, Kyoto University, Japan

Randy Snurr, Northwestern University, USA

Brigitte Stadler, Aarhus University, Denmark

Doros Theodorou, National Technical University of

Athens, Greece

Matthew Tirrell, University of Chicago, USA

Bernhardt L. Trout, MIT, USA

Raymond W.Y. Wong, Hong Kong

Polytechnic University, Hong Kong

Jia Zhu, Nanjing University, China

Meifang Zhu, Donghua University, China

Information for Authors

Full details on how to submit material for publication in MSDE are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/molecular-engineering. Submissions: The journal welcomes submissions of manuscripts for publication as Review Articles and Minireviews. Full Papers and Communications should describe original work of high quality and impact.

Additional details are available from the Editorial Office or

<http://www.rsc.org/authors>

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

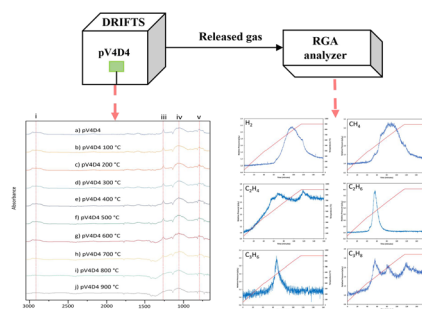
Registered charity number: 207890



1130

Time-resolved *operando* analysis of the pyrolysis of a PECVD-deposited siloxane polymer using a combined DRIFTS–MS system

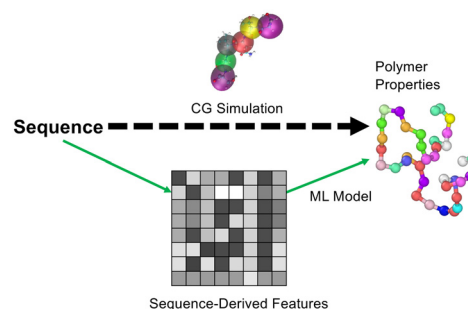
Bryan Nguyen, Farnaz Tabarkhoon, Linghao Zhao, Ankit Mishra, Malancha Gupta, Priya Vashishta and Theodore Tsotsis*



1146

Data-driven models for predicting intrinsically disordered protein polymer physics directly from composition or sequence

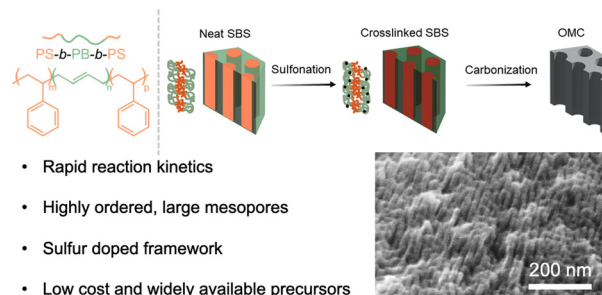
Tzu-Hsuan Chao, Shiv Rekhi, Jeetain Mittal and Daniel P. Tabor*



1156

Precursor design for efficient synthesis of large-pore, sulfur-doped ordered mesoporous carbon through direct pyrolysis

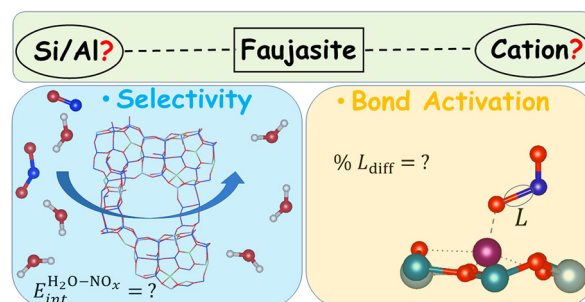
Mark Robertson, Anthony Griffin, Alejandro Guillen Obando, Andrew Barbour, Ryan Davis and Zhe Qiang*



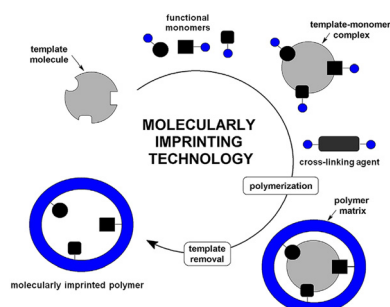
1165

A systematic DFT screening of cationic faujasite-type zeolites for the adsorption of NO, NO₂ and H₂O

Ioannis Karamanis, Ayoub Daouli, Hubert Monnier, Marie-Antoinette Dziurla, Guillaume Maurin and Michael Badawi*



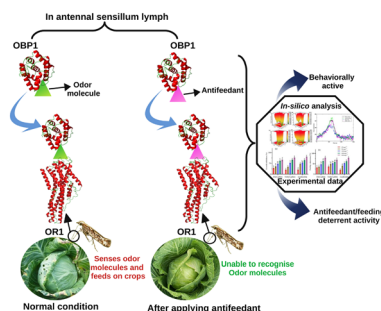
1182



Theoretical design of molecularly imprinted polypyrrole biosensor for the detection of renal failure biomarkers

Elham Rajaei, Mohammad Izadyar* and Mohammad Reza Housaindokht

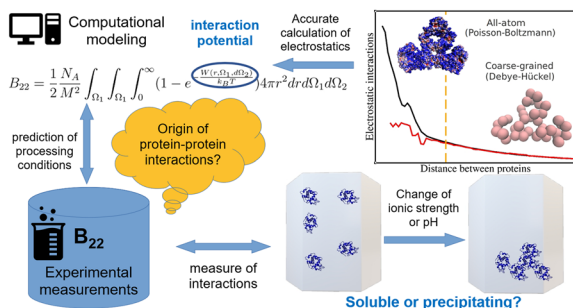
1195



Bioactive molecules of *Triadica sebifera* as eco-friendly antifeedants against *Plutella xylostella*: a pest management approach

Rahul Singh, Vijay Kumar Bhardwaj, Shudh Kirti Dolma, Sandeep Kumar, S. G. Eswara Reddy* and Rituraj Purohit*

1203



Accurate calculation of second osmotic virial coefficients of proteins using mixed Poisson-Boltzmann and extended DLVO theory

Srdjan Pusara, Wolfgang Wenzel and Mariana Kozłowska*

